Theoretical and Computational Methods for Fresnel Diffractive Imaging.

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Conventional approaches to coherent diffractive X-ray imaging are based on the assumptions of plane-wave illumination of the sample and weak X-ray scattering described by the first Born approximation. The retrieval of complex electromagnetic wavefields from oversampled far-field diffraction data and *a priori* information about the finite support of the diffracting object using iterative projective algorithms is now a well-established computational procedure. The convergence of these schemes is often poor because the operators that define such schemes do not represent projections onto convex sets and, viewed as a problem in optimization theory, minimization of the error involved in fitting the diffracted intensities leads to multiple minima and iterative stagnation. A range of relaxation schemes has been proposed that provide practical, and frequently successful, solutions to the stagnation problem, but the formal non-convex structure of the underlying inverse problem remains. In addition, the use of plane-wave illumination necessitates the use of beam stops to protect the detector, resulting in a loss of some small-angle scattering information that plays an important role in determining the overall normalization of the wave.

The Centre for Coherent X-ray Science has developed techniques that employ illumination structured in both phase and amplitude. Experiments based on this approach generate both a low-resolution holographic signal as well as large-angle scattering data carrying high-resolution structural information. No small-angle scattering information is lost, because beam stops at the detector plane are not required. The phase structure of the illumination removes the transverse translational degrees of freedom inherent in far-field Fraunhofer diffraction, and profoundly changes the mathematical and computational characteristics of existing phase retrieval algorithms.

This presentation examines the theoretical and computational advantages inherent in the use of illumination possessing phase structure, including the effect on conventional projective iterative methods such as the Error Reduction, Hybrid-Input-Output and Difference Map algorithms. We explore the use of approximate solutions of the Transport of Intensity equation to provide initial trial functions for these iterative algorithms and demonstrate how reconstruction ambiguities may be resolved by employing independent solution algorithms in parallel. The hypersurface in the active parameter space characterizing the mean-square fitting error in fitting the experimental data is finally examined in the context of the modification caused by the application of phase curvature to the sample, demonstrating the dramatic reduction in the density of local minima and the increased likelihood of finding a solution corresponding to the global error minimum.